



NORMAN L. ALLINGER

# A Portrait of the Chemist: The Lou Allinger Story

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Just about everyone these days is writing biographies of famous people, preparing commentaries on newsworthy events, or making movies on historical events. Typically, they are paid handsomely for their efforts. Careful investigation of these self-proclaimed experts more often than not reveals that they totally lack any credible journalistic or historical credentials. So is the case of this writing, except that I am not expecting significant—for that matter, any—financial remuneration.

My claim to the distinction and honor of being asked to write a summary of the career and achievements of Professor Norman L. Allinger can be traced to the fact that I am a friend and colleague—and I have pictures. More on the pictures later. Lou and I have worked closely together over the years, and he has been my computational chemistry mentor.

When the symposium to honor Professor Allinger was in the planning stages, Professors Henry "Fritz" Schaefer and Paul von R. Schleyer both came into my office one day. I was asked if I would participate in the proposed symposium and give a presentation. I told both of my senior colleagues that I would be honored and that I had a number of interesting molecular modeling projects that would be appropriate for such an event and suitable for publication in a special edition of the *Journal of Computational Chemistry*. They looked at one another and then told me that they wanted me to kick off the event! I was told that my lecture would be the most important one and set the tone for the whole meeting. I was deeply honored, but in the back of my mind I imagined that my South-

ern ancestors had been told similar things just before they made that fateful charge in 1863 at Gettysburg. My presentation was suppose to be accurate, highly illuminating, informative, eye-opening, and punctuated with humor. In other words, a typical Phil Bowen lecture.

By the time Fritz and Paul finished pumping me up and left my office, I, like my ancestors, was ready to make the charge and start shooting, and in this case I knew the first two who would be likely targets. Giving an introduction—with humor—is a difficult undertaking, but I had pictures. Earlier, Lou had been awarded the American Chemical Society Award for Computers in Chemical and Pharmaceutical Research. Kenny Lipkowitz, who was going to present the award and introduce Lou at the New Orleans ACS meeting, telephoned me in my office and asked if I knew of any interesting—or was the word *incriminating*—pictures. I turned to Lou's efficient secretary, Shawn, and his lovely wife, Irene, for assistance. A set of pictures was found, slides were prepared and sent off to Kenny, and I had the presence of mind to keep an extra set for the appropriate occasion, and this was it.

The following comments are loosely based on the presentation I made.

Professor Norman L. Allinger is a native Californian. Lou was born on April 6, 1928, and will soon be celebrating his 70th birthday. He likes to tell people that he was born and reared on a small island in San Francisco Bay. This usually leaves people with a number of questions. It took me a few years to ask him which island. The most

famous island, of course, is Alcatraz, but I did not want to pry into his early years. I was relieved to learn that there are other islands besides Alcatraz in San Francisco Bay.

Professor Norman L. Allinger, as we all know, has been a strong driving force in the creation of an entirely new specialty in chemistry and is widely recognized for his pioneering work and popular computer programs. He is widely recognized in both the academic and industrial communities for his seminal contributions in the area of theoretical organic chemistry. He has been at the forefront of development and applications of computational chemistry from the very beginning of the computer age.

Lou received his Ph.D. in 1954 at the University of California, Los Angeles, after having received his B.S. in chemistry in 1951 at the University of California, Berkeley. Originally Lou was trained as an experimental organic chemist under the direction of Professor Donald Cram. Prior to and during his studies, Lou earned a living as a professional New Orleans style jazz pianist. From time to time even today, he plays a few bars in the lab where a piano is ready and waiting.

His first of more than 360 published papers appeared in the chemical literature more than 40 years ago.<sup>1</sup> He was probably the first organic chemist to describe in the chemical literature a computer program written to solve a problem in organic chemistry.<sup>4</sup>

He did postgraduate research as an NSF Postdoctoral Fellow at Harvard University (1955–1956). His first academic appointment was at Wayne State University (1956–1968), where he quickly advanced in the ranks to full Professor. In 1968, he moved his research group to the University of Georgia, which has been his home ever since.

There are just too many awards and honors to list them all. He is highly sought after as an industrial consultant and has been invited to lecture throughout the world. He is one of only two chemists in the state of Georgia who is a member of the National Academy of Sciences. He was the recipient of the 1988 Arthur C. Cope Scholarship Award and the 1989 James Flack Norris Award in Physical Organic Chemistry from the American Chemical Society, and as mentioned above he was the 1996 recipient of the ACS Award of Computers in Chemistry & Pharmaceutical Research. He was an Alfred P. Sloan Research Fellow (1958–1960), and was elected in 1985 as an honorary member of the Serbian Chemical Society, and is listed in *Who's Who in America* and *Outstanding Personalities of the*

*South*. He was recently given an honorary doctorate by the Russian Academy of Sciences.

Professor Allinger's publications are heavily cited. In 1956, following his earlier work in natural products and synthesis (including the first use of NMR spectroscopy in the determination of the molecular structure of an organic natural product,<sup>2</sup> he became interested in conformational analysis. A series of papers<sup>3,5–7</sup> on this subject followed that emphasized the use of spectroscopic methods for studying molecular structure, and much of this work was summarized when the field was surveyed in the book *Conformational Analysis* by E. L. Eliel, N. L. Allinger, S. J. Angyal, and G. A. Morrison. Interestingly, Professors Eliel and Allinger have collaborated on a number of editorial projects, but, to my knowledge, have never published any original research papers together. Prior to conformational analysis being widely taught in graduate and undergraduate chemistry courses, they taught this material in the very first group of ACS short courses. Eventually, as the subject of conformational analysis began to be taught at the undergraduate level on a routine basis, the demand for the course disappeared. Since 1989, Lou has been involved in another popular ACS short course that highlights computational chemistry and molecular modeling methods. While this material also is beginning to be taught routinely at the graduate level in most institutions, the short course is still going strong.

In 1960, he began to apply quantum mechanics to practical problems in organic chemistry.<sup>8,9,12</sup> As computers became more powerful, he put them to use in quantum calculations of molecular properties such as electronic spectra,<sup>9,14</sup> optical rotary dispersion, and other properties related to conformation.<sup>12–14</sup> It was in the mid-1960s that he became interested in the development and applications of molecular mechanics.<sup>10</sup> Today he is considered the preeminent expert in this field.

It is noteworthy that one of his publications has been listed in Current Contents as a Citation Classic ("Conformational Analysis. LXIX. An Improved Force Field for the Calculation of the Structures and Energies of Hydrocarbons") having been cited in over 450 publications. Also, another one of his papers ("Calculation of Molecular Structures and Energy by Force Field Methods," *Advances in Physical Organic Chemistry*, Vol. 13, V. Gold and D. Bethell, Eds., Academic Press, New York, 1976) was chosen by the Citation Index as one of their most frequently cited papers.

Lou is the founder and editor of the *Journal of Computational Chemistry*. According to the Citation Index, this is a core journal in physical chemistry and chemical physics. Moreover, his popular book, *Molecular Mechanics*, is widely recognized as the authoritative treatment of molecular mechanics.

In summary, Professor Allinger has been a tireless champion of the use of conformational analysis and theoretical methods in organic chemistry.<sup>5-25</sup> His work, particularly in the area of molecular mechanics, has made it possible for pharmaceutical, agricultural, polymer, and biotechnology companies to initiate ambitious computer design programs. He has been a leader in helping to establish computational chemistry, especially molecular mechanics, as a standard research tool in organic chemistry through his insightful research and dedication to educational efforts. Anyone who knows Lou Allinger recognizes the breath of his imagination, the depth of his scholarship, the impact of his work, and his genuinely humble nature.

## Selected Papers

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